Unusual Hidden Symmetries in the t_{2g} Cubic Perovskites and the Magnetic Structure of LaTiO₃

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Abstract

The transition metal oxides have been the source of many fascinating physical phenomena such as high T_c superconductivity, colossal magnetoresistance, and orbiton physics. These surprising and diverse physical properties arise from strong correlation effects in the 3d bands. Most theoretical attempts to understand such systems are based on the Hubbard model. We recently show that [1, 2] for high symmetry transition metal oxides with threefold t_{2q} bands, this model possesses several novel hidden symmetries, which we use to prove that this model does not support long-range spin order at nonzero temperatures – despite the three-dimensional lattice structure. Introduction of spin-orbit coupling does allow spin ordering, but even then the excitation spectrum is gapless due to a subtle continuous symmetry [1, 2]. Thus, the experimentally observed spin order, with a gapped spectrum, of LaTiO₃ requires additional deviations from the simple Hubbard model. The main source of such deviations are the significant tilting of the TiO₆-octahedra and the small JT distortion which removes the degeneracy of the t_{2q} orbitals. We discuss the effects of these symmetry lowering terms and perform a super-exchange perturbation calculation for the magnetic Hamiltonian, including spin-orbit interaction on the Ti. The resulting magnetic structure is presented. This structure has mainly the G-type antiferromagnetism along the a axis of the orthorhombic structure, with a small ferromagnetic moment along the c axis, and a small A-type antiferromagnetic moment along the b axis.

References

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